

201-14932A

HIGH PRODUCTION VOLUME (HPV)

CHALLENGE PROGRAM

TEST PLAN

For

Nitric Acid, 2-Ethylhexyl Ester

**Prepared by
The American Chemistry Council
Petroleum Additives Panel
Health, Environmental, and Regulatory Task Group**

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**LIST OF MEMBER COMPANIES IN THE
HEALTH, ENVIRONMENTAL AND REGULATORY TASK GROUP**

The Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council Petroleum Additives Panel include the following member companies:

Chevron Oronite Company, LLC

Crompton Corporation

Ethyl Corporation

Groupe SNPE

ExxonMobil Chemical Company

Ferro Corporation

Infineum

The Lubrizol Corporation

Rhein Chemie Corporation

Rhodia, Inc.

1.0 INTRODUCTION

In March 1999, the American Chemistry Council (formerly the Chemical Manufacturers Association) Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG), and its participating member companies committed to address certain chemicals listed under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. This test plan follows up on that commitment. Specifically, this test plan sets forth how the HERTG intends to address testing information for the following substance: Nitric Acid, 2-Ethylhexyl Ester (2-EHN) (CAS No.: 27247-96-7)

In preparing this test plan the following steps were undertaken:

Step 1: A review of the literature and confidential company data was conducted on the physicochemical properties, mammalian toxicity endpoints, and environmental fate and effects for 2-EHN, using its CAS number, CAS name, and synonyms. Searches included the following sources: MEDLINE, BIOSIS, CANCERLIT, CAPLUS, CHEMLIST, EMBASE, HSDB, RTECS, EMIC, and TOXLINE databases; the TSCATS database for relevant unpublished studies on these chemicals; and standard handbooks and databases (e.g., Sax, CRC Handbook on Chemicals, IUCLID, Merck Index, and other references) for physicochemical properties.

Step 2: The compiled data was evaluated for adequacy in accordance with the EPA guidance documentation.

2.0 GENERAL SUBSTANCE INFORMATION

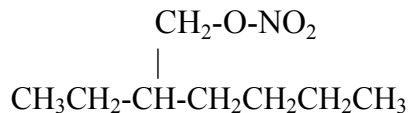
The substance that is the subject of this test plan is used as a fuel additive in diesel fuels. The chemical name, CAS Registry Number, molecular weight and chemical structure for this substance are presented below.

Chemical Name: Nitric acid, 2-ethylhexyl ester (2-EHN)

Chemical Abstract Service Registry Number: 27247-96-7

Molecular Weight: 175.2 g/mol

Chemical Structure:



3.0 EXPOSURE INFORMATION

Manufacture

A 50/50 mixture of undiluted Nitric and Sulfuric Acids is fed to a reaction tank along with a stoichiometric amount of 2-Ethylhexanol. The formation of the 2-EHN is almost instantaneous.

The reaction equation is as follows:



Any residual water is removed by passing the material through alumina bead dryers. The final 2-EHN product is then filtered and sent to storage.

Use

2-EHN is used as an ignition improver additive in diesel fuels to raise the cetane number.

4.0 PHYSICOCHEMICAL PROPERTIES

4.1 Summary of Available Data

Chemical and physical properties compiled by an industry consortium for 2-EHN are listed below. These data are drawn from technical data sheets, material data sheets, and IUCLID submissions.

Flash point	>70°C (closed cup)
Freezing point	<-45°C
Boiling point	>100°C (decomposes)
Vapor pressure	27 Pa @ 20°C
Vapor pressure	40-53 Pa @ 40°C
Vapor pressure	1.33 kPa @ 82°C
Density	0.96 g/ml @ 20°C
Solubility in water	12.6 mg/L @ 20°C
Lower explosive Limit	0.25% v/v in air (literature value – source u
Decomposition temperature	100°C

4.2 Data Assessment and Test Plan for Physicochemical Properties Relevant to Environmental Fate

2-EHN is a liquid at ambient temperatures (thus melting point is not-applicable). This substance undergoes a self-accelerating decomposition reaction if heated above 100°C. This exothermic reaction can become extremely violent and can ultimately end in an explosion. Therefore, the boiling point of this substance is not applicable. The vapor pressure of 2-EHN is 27 Pa @ 20°C, the water solubility is 12.6 mg/L @ 20°C. The octanol/water partition coefficient of 2-EHN has been reported to be 4.1. However no test report is available. Therefore, this parameter will be confirmed by QSAR modeling.

5.0 ENVIRONMENTAL FATE DATA

5.1 Biodegradability

5.1.1 Summary of Available Data

No adequate reliable published or unpublished biodegradation data on 2-EHN were located.

5.1.2 Data Assessment and Test Plan for Biodegradability

Biodegradation testing will be conducted.

5.2 Hydrolysis

5.2.1 Summary of Available Data

2-EHN was shown to hydrolyze in each of the pH conditions tested (pH 4, 7 and 9 at 25 and 50 °C). The mean half-life of the compound and water reaction at 25 °C ranged from 370 hours (pH 4.0) to 108 hours (pH 9.0)

5.2.2 Data Assessment and Test Plan for Hydrolysis

Hydrolysis testing will not be conducted.

5.3 Photodegradation

5.3.1 Summary of Available Data

No adequate published or unpublished photodegradation studies were located for 2-EHN .

5.3.2 Data Assessment and Test Plan for Photodegradation

The Atmospheric Oxidation Potential (AOP) of this substance will be characterized using the modeling program AOPWIN.

5.4 Fugacity Modeling

5.4.1 Summary of Available Data

There is no published or unpublished fugacity-based multimedia fate modeling data for 2-EHN.

5.4.2 Test Plan for Fugacity

The relative distribution of 2-EHN among environmental compartments will be evaluated using Level I Fugacity modeling.

6.0 ECOTOXICOLOGY DATA

6.1 Aquatic Ecotoxicity Testing

6.1.1 Summary of Available Data

2-EHN was evaluated for aquatic toxicity in fish, invertebrates and algae. In an acute aquatic toxicity study, conducted in Zebra fish, the 24, 48, 72 and 96 hour LC50s were >12.6 mg/L. In an acute daphnia study, the 24 and 48 hour EC50s were >12.6 mg/L. The 24 and 48 hour daphnia NOECs were >10 mg/L. In an acute algae toxicity test, the 72-hour no observed effect concentration, based on growth rate and growth inhibition, was 12.6 mg/L.

6.1.2 Data Assessment and Test Plan for Acute Aquatic Ecotoxicity

Adequate and reliable acute aquatic fish, invertebrate and algae toxicity studies were performed with 2-EHN. Additional aquatic ecotoxicity testing will not be conducted.

7.0 MAMMALIAN TOXICOLOGY DATA

7.1 Acute Mammalian Toxicity

7.1.1 Summary of Available Data

Acute oral and dermal toxicity studies are available for 2-EHN. In these studies, the LD₅₀ was greater than 10 mL/kg by the oral route and greater than 5 mL/kg by the dermal route indicating a low concern for toxicity.

7.1.2 Data Assessment and Test Plan for Acute Mammalian Toxicity

Adequate and reliable acute oral and dermal toxicity tests were performed for 2-EHN. Additional acute mammalian toxicity testing will not be conducted.

7.2. Mutagenicity

7.2.1 Summary of Mutagenicity Data

A negative *Salmonella typhimurium* point mutation assay is available for 2-EHN.

7.2.2 Data Assessment and Test Plan for Mutagenicity Toxicity

An adequate and reliable *Salmonella typhimurium* point mutation assay is available for 2-EHN. A chromosomal aberration study will be conducted on 2-EHN.

7.3 Repeated-dose, Reproductive and Developmental Toxicity

7.3.1 Summary of Repeated-Dose Toxicity Data

2-EHN has been evaluated in two inhalation toxicity studies in rats (two weeks duration followed by 2-week recovery periods), in a 21 day dermal toxicity study in rabbits and in a 28

day oral toxicity study in rats. The no observed effect levels in the inhalation, dermal and oral toxicity studies were 42 ppm, >500 mg/kg (systemic) and 20 mg/kg respectively. There were no published or unpublished reproductive or developmental toxicity tests located for 2-EHN.

7.3.2 Data Assessment and Test Plan for Repeated-dose Toxicity

Adequate and reliable inhalation, dermal and oral repeat dose toxicity studies are available for 2-EHN. Additional repeat dose toxicity studies will not be conducted.

A reproduction/developmental toxicity study will be conducted.

8.0 SUMMARY

The following table summarizes the available data and proposed testing on 2-EHN .Table 1
**Summary Table of Available Data and Proposed Testing on
 Nitric Acid, 2-Ethylhexyl Ester**

CAS No.: 27247-96-7	Study Results	Testing Proposed
Physical/Chemical Characteristics		
<i>Melting Point</i>	Not Applicable	No
<i>Boiling Point</i>	Not Applicable (violently decomposes)	No
<i>Vapor Pressure</i>	27 Pa @ 20°C	No
<i>Water Solubility</i>	12.6 mg/L @ 20°C	No
<i>Partition Coefficient</i>	4.1	Yes
Environmental Fate		
<i>Biodegradation</i>	No Adequate Data Located	Yes
<i>Hydrolysis</i>	Hydrolysis occurred under all conditions evaluated.	No
<i>Photodegradation</i>	No Data Located	Modeling
<i>Fugacity</i>	No Data Located	Modeling
Ecotoxicity		
<i>Acute Toxicity to Fish</i>	24, 48, 72 and 96 hour LC50s: >12.6 mg/L	No
<i>Acute Toxicity to Invertebrates</i>	24 and 48 hour EC50s: >12.6 mg/L 24 and 48 hour NOEC: >10 mg/L	No
<i>Acute Toxicity to Algae</i>	72 hour NOEC: 12.6 mg/L	No
Mammalian Toxicity		
<i>Acute Toxicity</i>	Oral LD50: >10 mL/kg (rat) Dermal LD50: >5 mL/kg (rabbit)	No
<i>Repeated Dose Toxicity</i>	14 Day Inhalation NOEL: 42 ppm 21 Day Dermal NOEL: >500 mg/kg (systemic) 28 Day Oral NOEL: 20 mg/kg/day	No
<i>Developmental Toxicity</i>	No Adequate Data Located	Yes
<i>Reproductive Toxicity</i>	No Adequate Data Located	Yes
Genotoxicity		
<i>Gene Mutation</i>	Not Mutagenic	No
<i>Chromosomal Aberration</i>	No Adequate Data Located	Yes